Floquet Theory and Control of Quantum Materials

Intensive Lectures at Yokohama National University — Lecture Notes

Takashi Oka

2 Basic structure of Floquet theory

Under a time-periodic external field, energy is not conserved, but a discrete time-translation symmetry remains. From this symmetry we show that the time evolution separates into a "slow part" and a "fine motion within one period". The conclusion of this lecture is a single formula, $U(t) = P(t)\,\mathrm{e}^{-\mathrm{i}H_F t}$.

2.1 Setup and conventions [5 min]

We set $\hbar = 1$. The Hamiltonian has period T:

$$H(t+T) = H(t), \qquad \Omega = \frac{2\pi}{T}.$$

The time-evolution operator is

$$\mathrm{i}\partial_t \,|\Psi(t)\rangle = H(t)\,|\Psi(t)\rangle\,, \qquad U(t,t_0) = \mathcal{T}\exp\Big[-\mathrm{i}\int_{t_0}^{t} H(s)\,ds\Big],$$

and satisfies the composition law $U(t,t_0) = U(t,t_1)U(t_1,t_0)$. From the periodicity of H,

$$U(t+T,\, t_0+T) = U(t,t_0).$$

Below we write $U(t) \equiv U(t,0)$.

2.2 Floquet's theorem [10 min]

The one-period evolution $U(T)$ is unitary, so its eigenvalues are complex numbers of modulus 1:

$$U(T)\,|\alpha\rangle = \mathrm{e}^{-\mathrm{i}\varepsilon_\alpha T}\,|\alpha\rangle\,.$$

The real number ε_α is called the **quasienergy**.

Theorem

Solutions of the Schrödinger equation of the following form (Floquet states) form a complete set:

$$\boxed{|\Psi_\alpha(t)\rangle = \mathrm{e}^{-\mathrm{i}\varepsilon_\alpha t}\,|u_\alpha(t)\rangle\,, \qquad |u_\alpha(t+T)\rangle = |u_\alpha(t)\rangle\,.}$$

Proof

Define $|u_\alpha(t)\rangle \equiv \mathrm{e}^{\mathrm{i}\varepsilon_\alpha t}U(t)\,|\alpha\rangle$. Using $U(t+T) = U(t+T,T)\,U(T) = U(t)\,U(T)$,

$$|u_\alpha(t+T)\rangle = \mathrm{e}^{\mathrm{i}\varepsilon_\alpha(t+T)}U(t)\,U(T)\,|\alpha\rangle = \mathrm{e}^{\mathrm{i}\varepsilon_\alpha t}U(t)\,|\alpha\rangle = |u_\alpha(t)\rangle\,.$$

General solution

Since $\{|\alpha\rangle\}$ is a complete set, for any initial state

$$|\Psi(t)\rangle = \sum_\alpha c_\alpha\,\mathrm{e}^{-\mathrm{i}\varepsilon_\alpha t}\,|u_\alpha(t)\rangle\,, \qquad c_\alpha = \langle\alpha|\Psi(0)\rangle\,.$$

The coefficients c_α are time independent. Floquet states play the role of "stationary states" in periodically driven systems.

Correspondence with Bloch's theorem

	Crystal (space)	Periodic drive (time)
Symmetry	$x \to x + a$	$t \to t + T$
Eigenstate	$\mathrm{e}^{\mathrm{i}kx} u_k(x)$	$\mathrm{e}^{-\mathrm{i}\varepsilon t} u(t)$
Conserved quantity	crystal momentum k	quasienergy ε
Identification	$k \sim k + 2\pi/a$	$\varepsilon \sim \varepsilon + \Omega$
Fundamental domain	Brillouin zone	$-\Omega/2 < \varepsilon \le \Omega/2$

Only $\mathrm{e}^{-\mathrm{i}\varepsilon T}$ is determined, so ε is ambiguous by integer multiples of Ω.

Energy conservation is weakened to "quasienergy is conserved modulo Ω". The system can exchange energy with the external field in integer multiples of Ω (photons).

2.3 Stroboscopic evolution and micromotion [15 min]

Definitions

$$H_F \equiv \frac{\mathrm{i}}{T} \log U(T) = \sum_\alpha \varepsilon_\alpha \, |\alpha\rangle\langle\alpha| \,, \qquad P(t) \equiv U(t)\, \mathrm{e}^{\mathrm{i}H_F t} = \sum_\alpha |u_\alpha(t)\rangle\langle\alpha| \,.$$

H_F is called the **Floquet Hamiltonian**. Floquet's theorem can be restated as:

$$\boxed{U(t) = P(t)\, \mathrm{e}^{-\mathrm{i}H_F t}, \qquad P(t+T) = P(t), \quad P(0) = 1.}$$

- $\mathrm{e}^{-\mathrm{i}H_F t}$: the evolution seen only at times $t = nT$ (**stroboscopic evolution**). $U(nT) = \mathrm{e}^{-\mathrm{i}H_F nT}$, which is indistinguishable from the evolution under the time-independent Hamiltonian H_F.
- $P(t)$: the motion within one period (**micromotion**). It is invisible at $t = nT$.

Two ambiguities

1. **Branch of the logarithm**. $U(T)$ is unchanged under $\varepsilon_\alpha \to \varepsilon_\alpha + n_\alpha \Omega$. To fix H_F, we must choose the interval in which the quasienergies are taken (where to place the branch cut). $P(t)$ then changes as well.
2. **Time origin**. Starting from t_0 gives $H_F[t_0] = P(t_0) H_F P(t_0)^\dagger$. The spectrum is the same; the basis differs. A form that does not depend on the origin is

   $$U(t, t_0) = \mathrm{e}^{-\mathrm{i}K(t)}\, \mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}(t-t_0)}\, \mathrm{e}^{\mathrm{i}K(t_0)}, \qquad K(t+T) = K(t).$$

   H_{eff} is called the effective Hamiltonian and $K(t)$ the kick operator (next lecture).

Ambiguity 1 is absent in equilibrium systems. "Where to place the branch cut" plays the leading role in the anomalous Floquet phases of Lecture 5.

2.4 Simplest example: a free electron in an AC electric field [10 min]

Absorbing the charge into $\boldsymbol{A}$, we take $H(t) = (\boldsymbol{p} + \boldsymbol{A}(t))^2/2m$. Consider circularly polarized light $\boldsymbol{A}(t) = A(\cos\Omega t, \sin\Omega t)$. Since $\boldsymbol{p}$ is conserved and $H(t)$ at different times commute,

$$U(t) = \exp\Big[-\mathrm{i}\int_0^t \frac{(\boldsymbol{p} + \boldsymbol{A}(s))^2}{2m} ds\Big] = \underbrace{\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{\xi}(t)}}_{P(t)} \exp\Big[-\mathrm{i}\Big(\underbrace{\frac{p^2}{2m} + \frac{A^2}{2m}}_{H_F}\Big)t\Big],$$

$$\boldsymbol{\xi}(t) = \frac{1}{m}\int_0^t \boldsymbol{A}(s)\, ds = \rho\,(\sin\Omega t,\ 1 - \cos\Omega t), \qquad \rho = \frac{A}{m\Omega}.$$

- $P(t)$ is just a translation by $\boldsymbol{\xi}(t)$. The center of a wave packet is $\langle \boldsymbol{x} \rangle (t) = \boldsymbol{x}_0 + \boldsymbol{p}t/m + \boldsymbol{\xi}(t)$: uniform motion with a circular motion of radius ρ superposed.
- H_F is the free particle with only a constant $A^2/2m$ added.
- The center encloses an oriented area $\pi\rho^2$ per period. The time-averaged orbital magnetic moment is $\frac{1}{2}\overline{(\boldsymbol{r} \times \boldsymbol{v})_z} = \pi\rho^2/T$, i.e. (area)/$T$.
- For linearly polarized light $\boldsymbol{A} = A \sin \Omega t\, \hat{\boldsymbol{x}}$, the motion is a back-and-forth oscillation $\xi_x = \rho(1 - \cos \Omega t)$ and the area is 0. Then $H_F = p^2/2m + A^2/4m$. The constant $A^2/4m$ is the average kinetic energy of the quiver motion (ponderomotive energy).



circular linear (area 0)

For a free particle, the micromotion leaves only a constant in H_F. H_F changes in an essential way when there is (a) a lattice (non-parabolic dispersion) or (b) internal degrees of freedom (spin, sublattice) (next lecture). The "micromotion area" reappears in Lecture 5.

2.5 Sambe space [15 min]

$|u_\alpha(t)\rangle$ is periodic, so it can be Fourier expanded. The same holds for $H(t)$:

$$H(t) = \sum_m H_m \, \mathrm{e}^{-\mathrm{i}m\Omega t}, \qquad |u_\alpha(t)\rangle = \sum_m \mathrm{e}^{-\mathrm{i}m\Omega t} \, |u_\alpha^m\rangle \, .$$

Inserting $|\Psi_\alpha\rangle = \mathrm{e}^{-\mathrm{i}\varepsilon_\alpha t} \, |u_\alpha(t)\rangle$ into the Schrödinger equation gives $[H(t) - \mathrm{i}\partial_t] \, |u_\alpha(t)\rangle = \varepsilon_\alpha \, |u_\alpha(t)\rangle$. For each Fourier component,

$$\boxed{\sum_n \big(H_{m-n} - m\Omega \, \delta_{mn}\big) \, |u_\alpha^n\rangle = \varepsilon_\alpha \, |u_\alpha^m\rangle \, .}$$

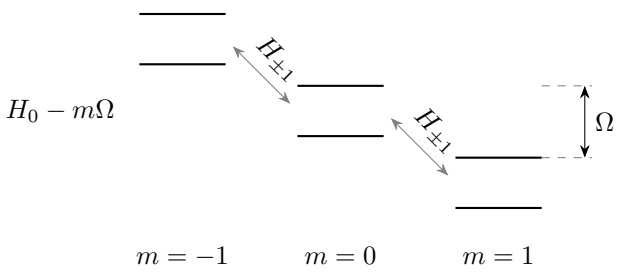
The time-dependent problem has become a time-independent eigenvalue problem. In matrix form (row m, column n),

$$\begin{pmatrix} \ddots & & & & \\ & H_0 + \Omega & H_{-1} & H_{-2} & \\ & H_1 & H_0 & H_{-1} & \\ & H_2 & H_1 & H_0 - \Omega & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ u^{-1} \\ u^0 \\ u^1 \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} \vdots \\ u^{-1} \\ u^0 \\ u^1 \\ \vdots \end{pmatrix} .$$

The original Hilbert space extended by the Fourier index m is called **Sambe space**.

Picture: a lattice in one higher dimension

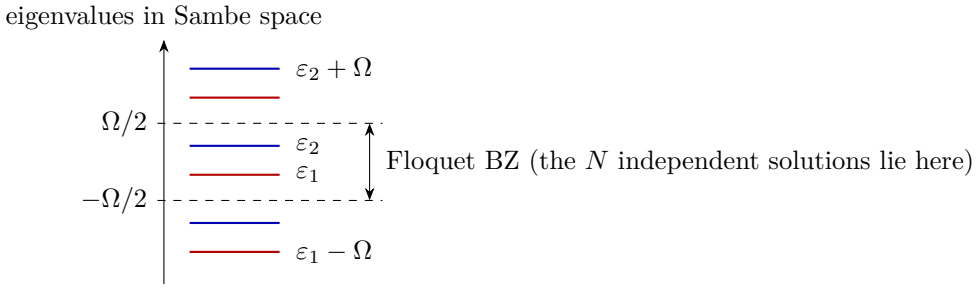
- m is the "number of absorbed photons". Regarded as a coordinate, m labels the lattice sites along a new direction.
- The diagonal term $-m\Omega$ is a uniform static electric field (tilted potential) in the m direction.
- $H_{\pm 1}$ is hopping to the neighboring layer (absorption/emission of one photon); $H_{\pm 2}$ is next-nearest-neighbor hopping.



A D-dimensional periodically driven system = a static D+1-dimensional system in a static electric field. The m direction is a "synthetic dimension" (the first column of the map in Lecture 6).

Redundancy

If $(\varepsilon, \{u^m\})$ is a solution, so is $(\varepsilon + n\Omega, \{u^{m+n}\})$, and it represents the same physical state $|\Psi(t)\rangle$. The spectrum in Sambe space repeats itself every Ω. Only the solutions within one Floquet BZ are independent. In numerical calculations, we diagonalize the matrix truncated at $|m| \le M$ and take the eigenvalues near the center.



Inner product

The inner product in Sambe space is the average over one period: $\langle\langle u|v\rangle\rangle = \frac{1}{T}\int_0^T dt\ \langle u(t)|v(t)\rangle = \sum_m \langle u^m|v^m\rangle$.

2.6 Content of the quasienergy [10 min]

Multiply $[H - \mathrm{i}\partial_t]\,|u_\alpha\rangle = \varepsilon_\alpha\,|u_\alpha\rangle$ by $\langle u_\alpha|$ and average over one period:

$$\varepsilon_\alpha = \underbrace{\frac{1}{T}\int_0^T dt\ \langle u_\alpha(t)|H(t)|u_\alpha(t)\rangle}_{\text{average energy}} - \underbrace{\frac{1}{T}\int_0^T dt\ \langle u_\alpha|\mathrm{i}\partial_t|u_\alpha\rangle}_{\gamma_\alpha\ \text{(geometric phase)}} \pmod{\Omega}.$$

γ_α is the Aharonov–Anandan phase (the Berry phase for non-adiabatic evolution). The quasienergy consists of the dynamical phase and the geometric phase of the closed path that the state traces in one period.

Hellmann–Feynman theorem

For a parameter λ,

$$\frac{\partial\varepsilon_\alpha}{\partial\lambda} = \frac{1}{T}\int_0^T dt\ \langle u_\alpha(t)|\frac{\partial H}{\partial\lambda}|u_\alpha(t)\rangle\,.$$

In particular, for $\lambda = k$ (wave number), $\partial\varepsilon_\alpha/\partial k$ is the velocity averaged over one period (used in Lecture 4).

Observables

Expectation values in a Floquet state are periodic in time: $\langle\Psi_\alpha(t)|O|\Psi_\alpha(t)\rangle = \langle u_\alpha(t)|O|u_\alpha(t)\rangle = \sum_m O_m \mathrm{e}^{-\mathrm{i}m\Omega t}$. $m = 0$ gives the time average, and $m \neq 0$ the response at harmonics of the external field (high-harmonic generation, etc.).

2.7 Example: spin in a rotating magnetic field and resonance [15 min]

$$H(t) = \frac{B_z}{2}\sigma_z + \frac{B_\perp}{2}\big(\sigma_x \cos\Omega t + \sigma_y \sin\Omega t\big).$$

In general, under a time-dependent unitary transformation $|\Psi\rangle = R(t)\left|\tilde{\Psi}\right\rangle$, the state $\left|\tilde{\Psi}\right\rangle$ obeys

$$\tilde{H} = R^\dagger H R - \mathrm{i} R^\dagger \partial_t R.$$

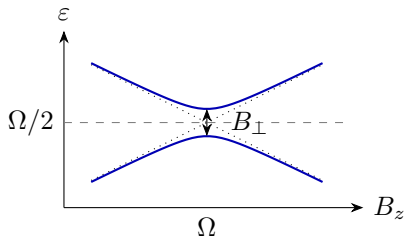
In the frame rotating with the magnetic field, $R(t) = \mathrm{e}^{-\mathrm{i}\Omega t\sigma_z/2}$, the Hamiltonian is time independent:

$$\tilde{H} = \frac{B_z - \Omega}{2}\sigma_z + \frac{B_\perp}{2}\sigma_x.$$

$\mathrm{e}^{-\mathrm{i}\Omega t\sigma_z/2}$ has period $2T$; reassigning a phase so that it becomes T-periodic gives

$$P(t) = \mathrm{e}^{-\mathrm{i}\Omega t(\sigma_z - 1)/2}, \qquad H_F = \tilde{H} + \frac{\Omega}{2}, \qquad \varepsilon_\pm = \frac{\Omega}{2} \pm \frac{1}{2}\sqrt{(B_z - \Omega)^2 + B_\perp^2}.$$

- At resonance $\Omega = B_z$, $\varepsilon_\pm = \Omega/2 \pm B_\perp/2$. A gap of width $B_\perp$ opens at the **boundary** $\Omega/2$ of the Floquet BZ.
- In Sambe space, $H_1 = \frac{B_\perp}{2}\sigma_+$ and $H_{-1} = \frac{B_\perp}{2}\sigma_-$. Only the pairs $(\uparrow, m)$ and $(\downarrow, m-1)$ are coupled, and the matrix splits into 2×2 blocks. These two levels cross at $B_z = \Omega$, and $H_{\pm 1}$ causes level repulsion.
- Rabi oscillation is the beating of a superposition of the two Floquet states (frequency $\varepsilon_+ - \varepsilon_-$).



Checking the content of the quasienergy

In the Floquet state $|u_+(t)\rangle = P(t)\,|+\rangle$, the spin rotates in sync with the magnetic field on a cone tilted from the z axis by an angle ϑ ($\tan\vartheta = B_\perp/(B_z - \Omega)$).

$$\gamma_+ = \int_0^T dt\ \langle u_+|\mathrm{i}\partial_t|u_+\rangle = -\pi(1 - \cos\vartheta) = -\frac{(\text{cone solid angle})}{2}, \qquad \overline{E}_+ = \frac{B_z\cos\vartheta + B_\perp \sin\vartheta}{2}.$$

$\varepsilon_+ = \overline{E}_+ - \gamma_+/T$ agrees with the result above. At resonance ($\vartheta = \pi/2$), $\gamma_+ = -\pi$, and the $\Omega/2$ in the quasienergy is nothing but the geometric phase π.

How the field is switched on

Take the initial state to be $|\uparrow\rangle$.

- **Sudden switch-on**: $c_\pm = \langle\pm|\uparrow\rangle$. At resonance $|c_\pm|^2 = 1/2$, and the two Floquet states are mixed equally. $\langle\sigma_z\rangle$ oscillates at frequency $B_\perp$.
- **Slow switch-on** (away from resonance): the state is adiabatically transferred to a single Floquet state, and no beating occurs.

Which Floquet state is occupied is determined by how the field is switched on. Adiabatic following breaks down at points where quasienergy levels cross (resonances).

Linearly polarized case

[optional] For $H' = B_\perp \sigma_x \cos\Omega t$, $H_{\pm 1} = \frac{B_\perp}{2}\sigma_x$, and $(\uparrow, m)$ couples not only to $(\downarrow, m-1)$ but also to $(\downarrow, m+1)$ (counter-rotating term). The blocks do not close and the problem cannot be solved exactly. A shift of the resonance position (Bloch–Siegert shift) and multiphoton resonances at $B_z \simeq 3\Omega, 5\Omega, \ldots$ appear.

2.8 Also periodic in space: Floquet–Bloch states [5 min]

When a spatially uniform external field is applied to a particle on a lattice, the wave vector $\boldsymbol{k}$ is conserved. Applying Floquet's theorem to $H(\boldsymbol{k}, t)$ at each $\boldsymbol{k}$ gives

$$\psi_{\alpha\boldsymbol{k}}(\boldsymbol{x}, t) = \mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x} - \varepsilon_\alpha(\boldsymbol{k})t)}\, u_{\alpha\boldsymbol{k}}(\boldsymbol{x}, t),$$

where u is periodic in both space and time. $\varepsilon_\alpha(\boldsymbol{k})$ is called a **Floquet–Bloch band**.

An equilibrium band $E(\boldsymbol{k})$ is periodic in $\boldsymbol{k}$, but E lies on the real line. A Floquet–Bloch band is **periodic in both $\boldsymbol{k}$** and ε. This difference is the starting point of Lecture 4.

2.9 Summary [5 min]

- The evolution of a periodically driven system decomposes as $U(t) = P(t)\,\mathrm{e}^{-\mathrm{i}H_F t}$. H_F describes the stroboscopic evolution and $P(t)$ the micromotion.
- The quasienergy is defined modulo Ω and forms the Floquet BZ. A resonance appears as a gap at the BZ boundary.
- In Sambe space, a periodically driven system becomes a static problem on a lattice in one higher dimension.

Note: Floquet states are a **basis** for the time evolution. Which Floquet states are actually occupied, and by how much, is a separate problem determined by the initial state, how the field is switched on, and the coupling to the environment (Lecture 6).